Ozone Productivity of Atmospheric Organics

Subcontractor

Coordinating Research Council

Principal Investigator

John H. Seinfeld
California Institute of Technology
104-44 Caltech
Pasadena, CA 91125
(818) 395-4100

DOE Project Manager

Michael Gurevich
U.S. Department of Energy
CE-332, MS 6A-116/Forrestal
1000 Independence Avenue, SW
Washington, D.C. 20585
(202) 586-6014

NREL Technical Monitor

Brent Bailey
NREL
1617 Cole Boulevard
Golden, CO 80401
(303) 275-4468

Subcontract Number

AF-2-12252-10

Performance Period

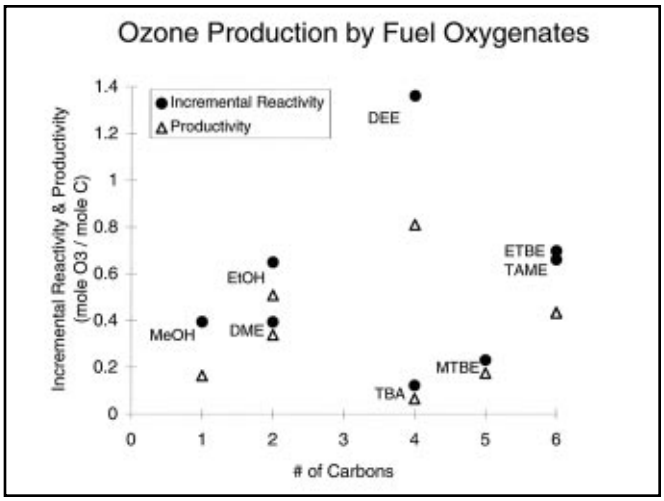
10/93–10/95

NREL Subcontract Administrator

Scott Montgomery (303) 275-3193

Objective

To determine the contributions to ozone (O_3) formation by individual volatile organic compounds (VOCs) in a complex VOC/oxides of nitrogen (NO_x) mixture and to examine the reactivity behavior of alternative fuels and reformulated gasoline (RFG) components.



Approach

A method that assigns O_3 or other product species back to the original organic precursors is used to unravel the complex chemistry of a mechanism. These results are used to explain the incremental reactivity behavior of individual VOCs, including components of RFG and alternative fuels.

Accomplishments

The assignment method for determining individual VOC contributions to O_3 formation has been developed and used to analyze trajectory model results. These studies have shown that the change in O_3 in an incremental reactivity calculation is caused by changes in O_3 production by all species present, not only the incremented organic. Among the eight fuel oxygenates tested, the species that contain only methyl or tertiary butyl groups such as methanol (MeOH) and methyl tertiary butyl ether (MTBE) were found to produce much less O_3 than those containing ethyl groups such as ethanol (EtOH) and ethyl tertiary butyl ether (ETBE).

Future Direction

We will evaluate the relationship between O_3 productivity and incremental reactivity for RFG and alternative fuel components.

Publications

Bowman, F.M. and J.H. Seinfeld. 1994. "Ozone Productivity of Atmospheric Organics," *J. Geophys. Res.*, 99, pp. 5309–5324.

Bowman, F.M. and J.H. Seinfeld. 1995. "Fundamental Basis of Incremental Reactivities," *Atmos. Environ.*, 28, pp. 3359–3368.

Bowman, F.M., C. Pilinis, and J.H. Seinfeld. 1995. "Ozone and Aerosol Productivity of Reactive Organics," *Atmos. Environ.*, 29 pp. 579–590.

Bowman, F.M. and J.H. Seinfeld. 1995. "Atmospheric Chemistry of Alternative Fuels and Reformulated Gasoline Components," Submitted to *Progress in Energy and Combustion Science.*